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FINAL TECHNICAL REPORT

Modeling and Numerical Methods for Material Growth and Convection

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Under support from this grant, substantial progress was made on a number of research projects, including the level set methods, modeling and simulation for material growth, Monte Carlo methods for rarefied gas dynamics, boundary value problem for Prandtl equations and image processing.

Level Set Methods.

Many problems in engineering design involve optimizing the geometry to maximize a certain design objective. Geometrical constraints are often imposed. In [7] we use the level set method, variational level set calculus, and the projected gradient method all developed at UCLA, to construct a simple numerical approach for problems of this type. We applied this technique to a model problem involving a vibrating system whose resonant frequency or whose spectral gap is to be optimized subject to constraints on geometry. The numerical results were quite promising. We expect to use this approach to deal with a wide class of optimal design problems in the future.

Applications include epitaxial crystal growth and image processing, as described below. R. Fedkiw and Stanley Osher wrote a comprehensive survey paper on level set and related methods [6]. In [9] we developed a fast approach to a local level set function.

Image Processing.

With H.-K. Zhao, B. Merriman and M. Kang [10] we considered a fundamental visualization problem: shape reconstruction from an unorganized data set. A new minimal-surface-like model and its variational and partial differential equation (PDE) formulation was introduced. In this formulation, only distance to the data set is used as the input. Moreover, the distance is computed with optimal speed using a new numerical PDE algorithm. The data set can include points, curves, and surface patches. The model has a natural scaling in the nonlinear regularization that allows flexibility close to the data set while it also minimizes oscillations between data points. To find the final shape, we continuously deform an initial surface following the gradient flow of our energy functional.

An offset (an exterior contour) of the distance function to the data set is used as our initial surface. A new and efficient algorithm to find this initial surface was developed. The level set method was used in numerical computation in order to capture the deformation of the initial surface and to find an implicit representation (using the signed distance function) of the final shape on a fixed rectangular grid. The variational/PDE approach using the level set method allows one to handle complicated topologies and noisy or highly nonuniform data sets quite easily. the constructed shape is smoother than any piecewise linear reconstruction. Moreover, the approach is easily scalable for different resolutions and works in any number of space dimensions.

T. Chan, Osher and J. Shen obtained a digitized total variation filter for nonlinear denoising. This method is simple to describe and demonstrates the effectiveness and robustness of the TV method for image processing. This is described in [2] With A. Marquina we obtained fast and effective level set based TV restoration of images algorithms [5].

Epitaxial Crystal Growth.

Our island dynamics model for epitaxial crystal growth and the level set method for its simulation has been very successful. Development of this method and stability analysis is contained in the papers of Cafilisch and co-workers.

We greatly improved the efficiency and applicability of both the numerical methods and the model in our level set approach to thin film epitaxial growth. The numerical method is described in the paper [3]. Analysis of the model for epitaxial growth is in [1].

We also have incorporated or started to incorporate a number of additional physical phenomena into the method, including detachment at step edge boundaries, edge diffusion, finite lattice size effects and elastic strain. These are making the method much more accurate and robust.

Prandtl equations.

Cafilisch and co-workers have analyzed the structure of boundary layers for the Navier-Stokes and Prandtl equations in [4].

Implicit Monte Carlo Methods for Rarefied Gas Dynamics (RGD).

Rarefied gas flows occur in a wide range of problems from space flight, material growth and other applications. In material processing, for example, rarefied flows occur in the boundary layers near the growth surface in CVD, sputtering, or other systems. Currently the method of choice for simulation of rarefied is the Direct Simulation Monte Carlo (DSMC) method. This method requires time steps that are less than the collisional time scale. In the fluid dynamic limit, the collisional time scale goes to zero, but the actual time scale for variation of the flow is the fluid dynamic time scale, which is much longer. As a result, the DSMC method is very slow in many applications.

We have made significant progress in overcoming this basic difficulty. In particular, we have developed an implicit formulation for the nonlinear Boltzmann equation for RGD and a hybrid representation of the density function. Together, these allow for large time steps in the fluid dynamic regime. So far this has been worked out only for the spatially homogeneous problem, i.e. for the collisional step only, but we expect to extend it to the

fully spatially inhomogeneous problem by combining it with a particle advection method. This work appeared in [8].

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Russel Caflisch

Stanley Osher

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